

091393,527

(FILE 'HOME' ENTERED AT 09:55:02 ON 04 SEP 2003)

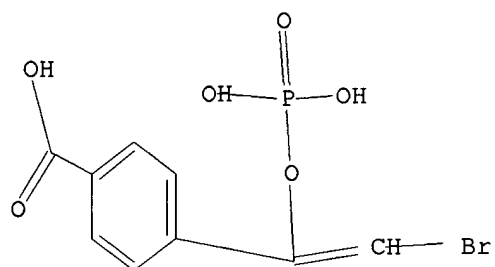
FILE 'REGISTRY' ENTERED AT 09:55:12 ON 04 SEP 2003

L1 STRUCTURE UPLOADED
L2 0 S L1 SSS FULL

=> d 11

L1 HAS NO ANSWERS

L1 STR

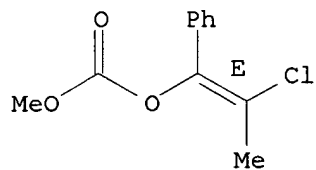


G1 Cb,Cy,Ak

Structure attributes must be viewed using STN Express query preparation.

L7 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN **136454-49-4** REGISTRY
CN Carbonic acid, 2-chloro-1-phenyl-1-propenyl methyl ester, (E)- (9CI) (CA
INDEX NAME)
FS STEREOSEARCH
MF C11 H11 Cl O3
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

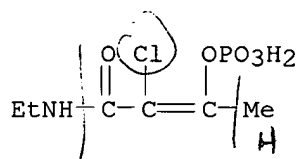
102

L2 ANSWER 1 OF 1 CAOLD COPYRIGHT 2002 ACS
 AN CA57:7553i CAOLD
 TI toxicology and pharmacology of a systemic phosphoric acid ester
 insecticide phosphamidon
 AU Jaques, Roland; Bein, H. J.
 IT 15844-87-8 89490-23-3

=> d l1 all

YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
 RN 89490-23-3 REGISTRY
 CN Crotonamide, 2-chloro-N-ethyl-3-hydroxy-, phosphate (7CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C6 H11 Cl N O5 P
 LC STN Files: CAOLD



crotonamide - phosphate

Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	3		(1) ACD
logD (LOGD)	-1.15	pH 1	(1) ACD
logD (LOGD)	-3.65	pH 4	(1) ACD
logD (LOGD)	-5.87	pH 7	(1) ACD
logD (LOGD)	-5.97	pH 8	(1) ACD
logD (LOGD)	-5.99	pH 10	(1) ACD
logP (LOGP)	-0.981+/-0.635		(1) ACD
Molar Solubility (SLB.MOL)	>=0.1 - <1 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	243.58		(1) ACD
pKa (PKA)	1.32+/-0.10	Most Acidic	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2002 ACD)

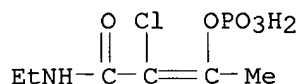
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 1 OF 1 CAOLD COPYRIGHT 2002 ACS
 AN CA57:7553i CAOLD
 TI toxicology and pharmacology of a systemic phosphoric acid ester
 insecticide phosphamidon
 AU Jaques, Roland; Bein, H. J.
 IT 15844-87-8 **89490-23-3**

=> d l1 all

YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
 RN **89490-23-3** REGISTRY
 CN Crotonamide, 2-chloro-N-ethyl-3-hydroxy-, phosphate (7CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C6 H11 Cl N O5 P
 LC STN Files: CAOLD



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
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H acceptors (HAC)	6		(1) ACD
H donors (HD)	3		(1) ACD
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logP (LOGP)	-0.981+/-0.635		(1) ACD
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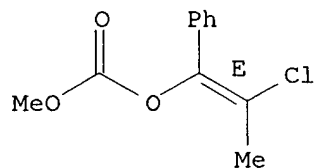
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS
 AN 1991:631804 CAPLUS
 DN 115:231804
 TI Reactions of polyhalo compounds with metals and electrophilic reagents.
 XII. Reactions of geminal .alpha.,.alpha.-dichloro-, .alpha.,.alpha.-
 dibromo-, and .alpha.,.alpha.-bromochloro-substituted ketones with zinc
 and acid chlorides
 AU Shchepin, V. V.; Gladkova, G. E.; Neifel'd, P. G.
 CS Perm. Gos. Univ., Perm, USSR
 SO Zhurnal Organicheskoi Khimii (1990), 26(11), 2394-7
 CODEN: ZORKAE; ISSN: 0514-7492
 DT Journal
 LA Russian
 CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 OS CASREACT 115:231804
 AB RCX₂COPh (R = Me, Et; X = Cl, Br) reacted with Zn and R₁COCl (R₁ = Me, Pr,
 Bu, Me₃C, PhCH₂, p-tolyl, MeO, p-ClC₆H₄OCH₂) in EtOAc at 40-45.degree. to
 give 18 corresponding RCX:CPhO₂CR₁ (I) as mixts. of E and Z isomers, with
 the former predominating, in 41-83% combined yield. EtCClBr₂COPh reacted
 under these conditions only at the C-Br bond, giving 61-69% I (R = Et, X =
 Cl; R₁ = Et, Pr, CMe₃).
 ST halo ketone reaction zinc acid chloride; ketone dihalo reaction zinc acid
 chloride; halophenylalkenyl ester; alkenyl ester halophenyl
 IT Carboxylic acids, esters
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (halophenylalkenyl esters, prepn. of, by reaction of dihaloalkyl Ph
 ketones with zinc and acid chlorides)
 IT Acid chlorides
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with zinc and dihaloalkyl Ph ketones, halophenylalkenyl
 esters by)
 IT Ketones, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (haloalkyl Ph, reaction of, with zinc and acid chlorides,
 halophenylalkenyl esters by)
 IT 54034-55-8P 54034-59-2P 73496-68-1P 136454-29-0P 136454-30-3P
 136454-31-4P **136454-32-5P** 136454-33-6P 136454-34-7P
 136454-35-8P 136454-36-9P 136454-37-0P 136454-38-1P 136454-39-2P
 136454-40-5P 136454-41-6P 136454-42-7P 136454-43-8P 136454-44-9P
 136454-45-0P 136454-46-1P 136454-47-2P 136454-48-3P
136454-49-4P 136454-50-7P 136454-51-8P 136454-52-9P
 136454-53-0P 136454-54-1P 136454-55-2P 136454-56-3P 136454-57-4P
 136454-58-5P 136454-59-6P 136480-44-9P 136509-08-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 IT 2114-03-6 57169-51-4 66255-85-4 66498-51-9 137853-30-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with zinc and acid chlorides, halophenylalkenyl ester by)
 IT 75-36-5, Acetyl chloride 79-22-1, Methyl chlorocarbonate 103-80-0,
 Phenylacetyl chloride 141-75-3, Butanoyl chloride 638-29-9, Pentanoyl
 chloride 874-60-2, p-Toluoyl chloride 3282-30-2, Pivaloyl chloride
 4122-68-3, (4-Chlorophenoxy)acetyl chloride
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with zinc and dihaloalkyl Ph ketones, halophenylalkenyl
 esters by)

=>

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INDEX NAME)
FS STEREOSEARCH
MF C11 H11 Cl O3
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
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Double bond geometry as shown.



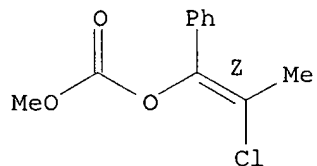
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1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

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L8 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN 136454-32-5 REGISTRY
CN Carbonic acid, 2-chloro-1-phenyl-1-propenyl methyl ester, (Z)- (9CI) (CA
INDEX NAME)
FS STEREOSEARCH
MF C11 H11 Cl O3
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

Double bond geometry as shown.



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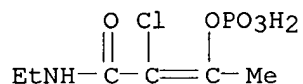
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 FS 3D CONCORD
 MF C6 H11 Cl N O5 P
 LC STN Files: CAOLD



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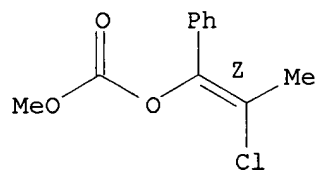
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